

two structures are strikingly very similar. Refinement of the structure by the Difference Synthesis is in progress.

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ON THE CRYSTAL STRUCTURE OF METHANOL AT -180°C

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The crystal structure of methanol has been studied by Tauer and Lipscomb (1952) by studying the Weissenberg and precession photographs of the crystal at -110°C and at -160°C . They reported that the crystal has a transition at -115°C the high temperature modification being orthorhombic conforming to the space group D_{2h}^{17} . The Weissenberg photographs taken for the crystal at -160°C show that the low temperature phase consists of small crystallites of low symmetry but not of a single crystal. They observed that the possible unit cell which accounts for all but a few weak reflections is monoclinic with two molecules in the unit cell having dimensions $a = 4.53 \text{ A.U.}$, $b = 4.69 \text{ A.U.}$, $c = 4.91 \text{ A.U.}$ and $\beta = 90^{\circ} \pm 3^{\circ}$. The space group C_{2h}^{28} was assigned to the crystal although they suggested the presence of some weak reflections indicating a super lattice. An attempt has been made to find out whether the crystal retains this symmetry at still lower temperatures upto -180°C .

The Debye-Scherrer pattern due to the crystal at -180°C was photographed by the method used earlier (Krishna Murti and Sen, 1956). The spacings calculated from the pattern obtained for the crystal at -180°C are given in Table I. The pattern has been analysed by trial and error method and it has been found that the crystal is monoclinic with the unit cell dimensions as $a = 4.59 \text{ A.U.}$, $b = 4.68 \text{ A.U.}$, $c = 4.92 \text{ A.U.}$ and $\beta = 97^{\circ}30'$. The density of the crystal at -180°C

TABLE I
 Spacings of crystals of methanol

at -160°C (Tauer and Lipscomb, 1952)			at -180°C		
Indices	Calculated spacings in A.U.	Observed structure factor (F_o)	Observed spacings in A.U. and Intensities	Calculated	
				spacings in A.U.	Indices
001	4.90	<4	4.86 (m)	4.88	001
100	4.52	9	4.55 (w)	4.55	100
10 $\bar{1}$	3.41	18	3.56 (vw)	3.57	101
011	3.39	18	3.38 (s)	3.38	011
110	3.26	24	3.26 (vs)	3.26	110
101	3.24	18	3.13 (m)	3.13	101
			2.84 (w)	2.84	111
			2.60 (w)	2.60	111
002	2.45	5			
020	2.345	—	2.335 (m)	2.34	020
			2.28 (w)	2.28	201
				2.275	200
200	2.26	5			
021	2.115	<4	2.11 (w)	2.11	021
102	2.11	8		2.05	210
120	2.08	6	2.04 (w)	2.04	102
210	2.04	6		1.97	211
201	2.01	9	1.98 (vw)	1.96	201, 121
121	1.93	8			
121	1.90	8	1.87 (w)	1.87	112, 121
			1.82 (w)	1.81	211
022	1.695	4		1.69	022
21 $\bar{2}$	1.64	7	1.68 (w)	1.67	212
003, 220	1.63	4	1.63 (vw)	1.63	12 $\bar{2}$
					220, 003
212	1.53	7		1.52	300
103		6	1.51 (w)	1.51	113, 30 $\bar{1}$
300	1.51	4		1.485	031
031	1.49	7			
130	1.48	7	1.48 (w)	1.48	212, 130
301	1.46	6		1.47	103

is found to be 0.98. The number of molecules in the unit cell is two. The extinction of *oko* for *k* odd places this crystal in the space group C_{2h}^2 or C_2^2 . The agreement between the calculated and observed spacings is shown in Table I.

Thus the space group remains the same at -180°C , but the angle β increases slightly. This increase in the angle β and in the primitive translation along *a*-axis, with lowering of the temperature from -160°C to -180°C , explains the changes in the intensities of reflection observed for certain planes (Table I)

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